

Linear Response calculations of T_c

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First -principles calculations of the superconducting transition temperature T_c require accurate knowledge of the wavevector-dependent electron-phonon interaction parameter $\lambda(\mathbf{q})$. Previous methods for determining $\lambda(\mathbf{q})$ required the use of supercells (with \mathbf{q} a reciprocal lattice vector) to restore the periodicity of the distorted lattice. As a result, it was impractical to calculate $\lambda(\mathbf{q})$ except at a limited set of wavevectors \mathbf{q} which were of high symmetry. Recently, linear response techniques which eliminate the need for supercells were applied¹ to the calculation of the electron-phonon interaction, allowing the calculation of $\lambda(\mathbf{q})$ throughout the Brillouin zone. I will report on the application of these techniques to the pressure dependence of T_c in silicon and in other materials.

¹S.Y. Savrasov, D.Y. Savrasov, and O.K. Anderson, Phys. Rev. Lett. **72**, 372 (1994).

Work performed under the auspices of the U.S. Department of Energy by LLNL under contract no. W-7405-ENG-48.